# Phase transition in the Rényi-Shannon entropy of Luttinger liquids

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(Dated: January 19, 2013)

The Rényi-Shannon entropy associated to critical quantum spins chain with central charge $c = 1$ is shown to have a phase transition at some value $n_c$ of the Rényi parameter $n$ which depends on the Luttinger parameter (or compactification radius R). Using a new replica-free formulation, the entropy is expressed as a combination of single-sheet partition functions evaluated at $n-$ dependent values of the stiffness. The transition occurs when a vertex operator becomes relevant at the boundary. Our numerical results (exact diagonalizations for the XXZ and $J_1 - J_2$ models) are in agreement with the analytical predictions: above $n_c = 4/R^2$ the subleading and universal contribution to the entropy is $\ln(L)(R^2 - 1)/(4n - 4)$ for open chains, and $\ln(R)/(1 - n)$ for periodic ones (R=1 at the free fermion point). The replica approach used in previous works fails to predict this transition and turns out to be correct only for $n < n_c$. From the point of view of two-dimensional Rokhsar-Kivelson states, the transition reveals a rich structure in the entanglement spectra.

*Introduction.*— The entanglement entropy (EE) has become an important tool to probe and characterize many-body quantum states. In one-dimensional (1d) systems, the celebrated logarithmic divergence [1–4] of the von Neumann entropy of a long segment provides an efficient way to measure the central charge of a critical spin chain. In higher dimensions, EE can also be used to detect the presence of topological order [5], which is otherwise invisible to conventional local order parameters and correlation functions. Understanding how scales the EE of large subsystems has also opened a route to algorithms able to simulate efficiently these strongly interacting systems in $d > 1$ [6].

In this letter, we use a seemingly completely different entropy to probe the ground-state of quantum spin chains, the *Shannon entropy* (or configuration entropy). For a normalized state $|\psi\rangle$ and a Rényi index $n > 0$ it is defined as :

$$S_n = \frac{1}{1-n} \ln \left( \sum_i p_i^n \right) \quad p_i = |\langle i|\psi\rangle|^2 \quad (1)$$

where the states $|i\rangle$ form a basis of the Hilbert space. The basis states are chosen to be products of local states, and the Ising configurations ($|i\rangle = |\uparrow\uparrow\downarrow \cdots\rangle$, etc.) are the natural choice for the spin-$\frac{1}{2}$ systems we consider. This entropy was originally introduced as a mean to evaluate the EE in some particular two-dimensional (2d) states – the so called Rokhsar-Kivelson (RK) wave functions – and has allowed to investigate in details the EE at some some 2d conformal quantum critical points [7, 8]. We will interpret our results in terms of 2d entanglement spectra at the end, but we will otherwise mostly concentrate on the 1d spin chain point of view.

A particularly interesting situation is that of the spin-$\frac{1}{2}$ XXZ chain:

$$\mathcal{H} = \sum_i \left( S_i^x \cdot S_{i+1}^x + S_i^y \cdot S_{i+1}^y \right) + \Delta \sum_i S_i^z \cdot S_{i+1}^z \quad (2)$$

For a chain of length $L$, $S_n$ has a leading term proportional to $L$ followed by universal subleading contributions. If the chain is *periodic*, the first subleading term is of order $O(1)$ and was shown to be [7, 9] :

$$S_n^{\text{periodic}} = (\cdots)L + \ln(R) - \frac{\ln n}{2(n-1)}, \quad (3)$$

where $R$ is the compactification radius, related to the anisotropy $\Delta$ of the XXZ Hamiltonian ($R(\Delta)^2 = 2 - \frac{2}{\pi} \arccos(\Delta)$). With *open* boundary conditions the first subleading correction is also universal and takes the form of a logarithm of the length $L$ of the chain [8]:

$$S_n^{\text{open}} = (\cdots)L - \frac{1}{4} \ln(L), \quad (4)$$

which, in the 2d-RK language, confirms at $c = 1$ the arguments developed in [10] (from now on the term proportional to $L$ will be omitted).

In this letter we however show that these results are only correct below a critical value $n_c$ of the Rényi parameter. Using a replica-free formulation of the problem we prove that the Rényi parameter $n$ effectively modifies the compactification radius of the chain (in a sense to be defined latter), and that a phase transition takes place at $n = n_c$ when a (boundary) vertex operator becomes relevant. A central result concerns the location of this transition and the behavior of the entropy above $n_c$:

$$n_c = d^2/R^2 \quad (5)$$

$$S_{n>n_c}^{\text{periodic}} = \frac{1}{n-1} \left( n \ln R - \ln d \right) \quad (6)$$

$$S_{n>n_c}^{\text{open}} = \ln(L) \frac{n}{n-1} \left( \frac{R^2}{4} - \frac{1}{4} \right), \quad (7)$$

where $d$ is the degeneracy of the Ising configuration with the highest probability $p_{\max}$ in the ground state. At zero magnetization this configuration is $d = 2$-fold degenerate:

$$|i_{\max}\rangle = |\uparrow\downarrow\uparrow\downarrow \cdots \uparrow\downarrow\rangle \quad \text{or} \quad |i_{\max}\rangle = |\downarrow\uparrow\downarrow\uparrow \cdots \downarrow\uparrow\rangle. \quad (8)$$

*Compact free field.*— To understand this transition we adopt the 1+1 dimensional (Euclidian) point of view. At long distances, the model is described by a compactified "height field" $h(x, \tau)$ with Gaussian probabilities:

$$S[h] = \frac{\kappa}{4\pi} \int dx d\tau (\nabla h)^2 \qquad (9)$$

$$\mathcal{Z} = \int \mathcal{D}[h] \, \exp\left(-S[h]\right). \qquad (10)$$

where $\kappa$ is the stiffness, $r$ the compactification radius ($h \equiv h + 2\pi r$) and the physical Luttinger parameter (which fixes the decay exponents of the correlations functions) is $R = \sqrt{2\kappa} r$. For periodic (resp. open) chains $h$ lives on an infinitely long cylinder (resp. strip) of perimeter (resp. width) $L$. In this language, the microscopic configurations $|i\rangle$ are replaced by configurations $\phi(x) = h(x, \tau = 0)$ of the height field at $\tau = 0$. To evaluate the probability $p[\phi]$ we decompose the field $h$ into an harmonic function $h^\phi$ which satisfies the boundary condition $h^\phi_{\tau=0} = \phi$, and a "fluctuating" part $\delta h$ satisfying a Dirichlet boundary condition: $h = h^\phi + \delta h$ [22]. Exploiting the Gaussian form of the action and $\Delta h_\phi = 0$, the "classical" and "fluctuating" part decouple: $S[h] = S[h^\phi] + S[\delta h]$ and we get

$$p[\phi] = \exp(-S[h^\phi]) \frac{\mathcal{Z}^D}{\mathcal{Z}}, \qquad (11)$$

where $\mathcal{Z}^D$ is the partition function of the whole cylinder (resp. strip) with a Dirichlet defect line at $\tau = 0$ [23]. Now $p[\phi]$ is raised to the (possibly non-integer) power $n$

$$p[\phi]^n = \exp(-nS[h^\phi]) \left(\frac{\mathcal{Z}^D}{\mathcal{Z}}\right)^n, \qquad (12)$$

and make the observation that $\exp(-nS[h^\phi])$ is the Boltzmann weight in a system where the stiffness $\kappa$ has been replaced by $\kappa' = n\kappa$. From now on we explicitly keep track of the value of the stiffness $\kappa$ (as an index) and write:

$$\exp(-nS_\kappa[h^\phi]) = \exp(-S_{n\kappa}[h^\phi]) = p_{n\kappa}[\phi] \frac{\mathcal{Z}_{n\kappa}}{\mathcal{Z}^D_{n\kappa}}. \qquad (13)$$

So, Eq. 12 can be written as

$$(p_\kappa[\phi])^n = p_{n\kappa}[\phi] \left(\frac{\mathcal{Z}_{n\kappa}}{\mathcal{Z}^D_{n\kappa}}\right) \left(\frac{\mathcal{Z}^D_\kappa}{\mathcal{Z}_\kappa}\right)^n. \qquad (14)$$

Inserting this result in Eq. 1 and using the fact that the probabilities $p_{n\kappa}[\phi]$ are normalized, we get the main result of this section:

$$S_n = \frac{1}{1-n} \left[ \ln\left(\frac{\mathcal{Z}_{n\kappa}}{\mathcal{Z}^D_{n\kappa}}\right) - n \ln\left(\frac{\mathcal{Z}_\kappa}{Z^D_\kappa}\right) \right] \qquad (15)$$

If we assume $2n = p$ to be an integer the partition function $Z(n) = \sum p_i^n$ has a natural interpretation in terms of

$p$ half-infinite systems glued together at their edge, forming a "book" with $p$ sheets [11]. The derivation above, however, never assumes $2n$ to be an integer and is therefore different from the previous derivations involving a replica trick [8, 9]. $S_n$ has been reduced to ratios of standard partition functions with respectively free and Dirichlet boundary conditions at the boundary between upper ($\tau > 0$) and lower ($\tau < 0$) parts of the cylindric (or strip). The complications associated to $n$-sheeted surfaces [8, 9] have been avoided. For a compactified free field and the cylinder geometry, the ratio $g_D^2 = \mathcal{Z}^D_\kappa/\mathcal{Z}_\kappa$ is a well known "$g$-factor" [12, 13]:

$$g_D^2 = R^{-1} = (2\kappa r^2)^{-1/2}. \qquad (16)$$

Combining Eq. 15 and 16 we find:

$$S_n = \ln R - \frac{\ln n}{2(n-1)}, \qquad (17)$$

in agreement with Refs. [7–9, 14]. For the strip geometry, we also recover the $n$-independent result of Eq. 4 by applying the Cardy-Peschel formula [15] to Eq. 15, with four angles $\gamma = \pi/2$.

*Boundary phase transition.*— Eq. 15 is a combination of two $g$-factors and therefore probes the boundary of the system (the "bookbinding" in the book picture). The action at the lattice scale is not strictly Gaussian and other terms respecting the lattice symmetry and the periodicity $h \equiv h + 2\pi r$ are present, including vertex operators of the type $\cos(\frac{d}{r} h)$. At the boundary such an operator renormalizes to zero in the long distance limit if $d^2 > 2\kappa r^2$ [16]. Otherwise it would lock the field to a flat configuration with degeneracy $d$. But the Eq. 15 cannot be valid anymore in this locked/massive phase since its derivation assumes Gaussian probabilities. A boundary phase transition therefore takes place when the most relevant vertex operator become marginal in presence of a stiffness $\kappa' = n\kappa$ [24]. This gives the critical value of the Rényi index:

$$n_c = \frac{d^2}{2\kappa r^2}. \qquad (18)$$

In the case of the antiferromagnetic XXZ chain the two Ising configurations $|\uparrow\downarrow\uparrow\downarrow \cdots\rangle$ and $|\downarrow\uparrow\downarrow\uparrow \cdots\rangle$ become the ground-states when $\Delta \to \infty$, which shows that an operator with two minima is present at the microscopic level. Taking $2\kappa r^2 = R(\Delta)$ and $d = 2$, we find Eq. 5. We also note that the same argument applies to the $J_1 - J_2$ (or "zig-zag") chain, and to any Luttinger liquid phase with umklapp terms $\sim \cos(2h/r)$.[25]

In this locked phase, the universal contribution to $S_n$ is given by these $d$ configurations only, so that

$$S_{n>n_c} = \frac{1}{1-n} \ln\left[d(p_{\max})^n\right]. \qquad (19)$$

In the periodic case, $p_{\max}$ simply corresponds to $g_D^2 = \mathcal{Z}^D/\mathcal{Z}$ and we recover Eq. 6.
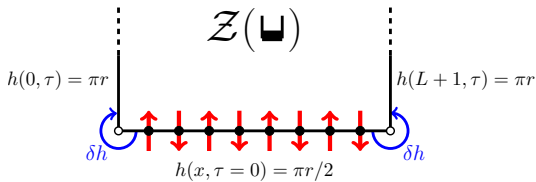
FIG. 1: (Color online) Height shift $\delta h = \pi r/2$ for the semi-infinite strip with bottom boundary condition $|i_{\max}\rangle$.

The open chains turn out to be even more interesting. The universal contribution to $S_{n>n_c}$ is encoded in

$$p_{\max} = \lim_{\tau \to \infty} \frac{\left|\langle s|e^{-\tau H}|i_{\max}\rangle\right|^2}{\langle s|e^{-2\tau H}|s\rangle} = \frac{\mathcal{Z}(\sqcup)^2}{\mathcal{Z}(||)}, \qquad (20)$$

where $\mathcal{Z}(\sqcup)$ is the partition function of a semi-infinite strip with bottom boundary condition $|i_{\max}\rangle$ (see Fig. 1). The ratio in Eq. 20 is similar, but not identical to the one used below the transition ($n < n_c$). As before, four corners with angle $\pi/2$ will contribute to $-\ln p_{\max}$ by a logarithm: $-\frac{1}{4}\ln L$. However, the configuration with highest probability does not exactly correspond to Dirichlet in the continuum limit since there is a *height shift* $\delta$ between the vertical edges of the strip, and the horizontal boundary (see Fig. 1). It can be treated by subtracting an harmonic function $h_\delta(x,\tau) = (2\delta/\pi)\arg(x+i\tau)$, equal to 0 on the horizontal boundary $\tau = 0$ and $\delta$ on the vertical boundary at $x = 0$. The resulting contribution to the free energy is

$$\delta F \sim \frac{\kappa \delta^2}{2\pi^2}\ln L. \qquad (21)$$

The value shift $\delta$ can be obtained using, for instance, a bosonization approach. The free boundary condition for the spins at the end of the open chain corresponds to Dirichlet for the free field and we have to set $h(x = 0,\tau) = h(x = L+1,\tau) = \pi r$ to insure vanishing spin operators at both ends [17]. Then, the continuum limit of the configuration $|i_{\max}\rangle$ corresponds to locking $h(x,\tau = 0)$ to the minima of the umklapp term $\cos(2h/r)$ [18], which has two degenerate minima in $h = \pi r/2$ and $3\pi r/2$. In both cases the height difference between the $x = 0$ boundary and that at $\tau = 0$ is $\delta = \pi r/2$. Summing up the contributions coming from Eq. 21 and from the Cardy-Peschel term, we recover our main result Eq. 7.

*Numerical simulations.*— So far, for periodic chains, only the case $n = 1$ has been investigated numerically [7]. Fig. 2 shows the full $n$ dependence of $S_n$ (constant term extracted by fitting the finite-size data) for different values of $\Delta$. Although the system sizes are very small ($L \leq 28$) there is a good agreement with the theoretical predictions, including the change of behavior at the predicted value of $n_c$ (which depends on $\Delta$). It is only close to the Heisenberg point ($\Delta = 1$) and above $n_c$ that the finite-size results deviate from Eq. 7. We attribute
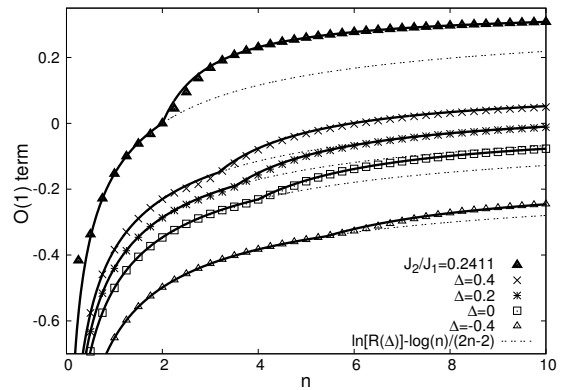


FIG. 2: Constant term in the Shannon-Rényi entropy of periodic XXZ and $J_1 - J_2$ chains for different values of $\Delta$ and at the critical point $J_2/J_1 = 0.2411$. Each point comes from fitting the data for $L = 20, 22, 24, 26$ and $28$ to $aL+b+c/L+d/L^2$. Fat lines: theoretical prediction (Eq. 15). Eq. 3 is also plotted above $n_c$ (dashed lines) for comparison.

these enhanced finite-size effects to the marginal operators present at the $SU(2)$ symmetric point. To circumvent this difficulty we also studied the $J_1 - J_2$ chain at the critical value $J_2/J_1 \sim 0.2411$ [19], which has the same radius $R = \sqrt{2}$ but where finite-size effects are much smaller. The data again agrees well with our prediction.

Open chains were investigated in Ref. [8] for various values of $n$ and $\Delta$, but the transition at $n_c$ was overlooked. In Fig. 3 we see a clear tendency for the logarithmic term to approach the theoretical curves, although the finite size data are still far from the thermodynamic limit. Interestingly, the entropies curves extracted from different system sizes cross in the immediate vicinity of the predicted value of $n_c$. This lead us to conjecture that the coefficient of the logarithm may take a universal value at the transition point which only depends on the compactification radius $R$. At $\Delta = 0$ we pushed the numerics to $L = 40$ spins (see below) and the inset of Fig 3 shows a collapse of the data for different system sizes onto a single curve in the vicinity of $n_c = 4$. This indicates a slow ($\sim L^{-1/4}$) but steady convergence towards a step function. We also get $S_{n=n_c}^{\text{open}} = -(1/6)\ln L$ with a high precision at $\Delta = 0$, although we have no theoretical understanding of this value.

$\Delta = 0$ *in open chains.*— This corresponds to free fermions and each probability $p_i$ is a determinant (Wick's theorem). Denoting by $\{x_k\}$ the positions of the up spins (fermions) and setting $\theta_k = \pi x_k/(L+1)$ we have:

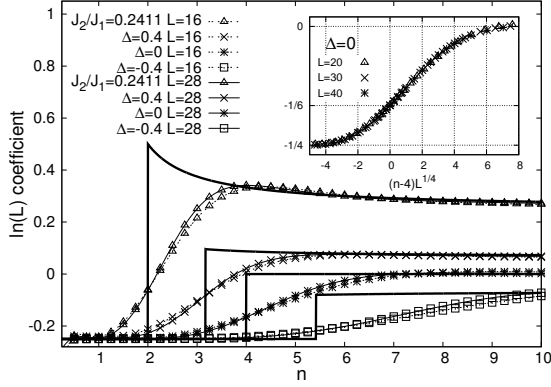$$p_i = p(\{\theta_k\}) = \left(\frac{2}{L+1}\right)^{L/4} \det_{1 \leq j,k \leq n}(\sin[j\theta_k]) \quad (22)$$

FIG. 3: Logarithmic term in the Shannon-Rényi entropy of open XXZ and $J_1 - J_2$ chains, extracted using a fit $aL + b \ln L + c + d/L$ to four consecutive even systems sizes $(L, \cdots, L-6)$ with $L = 16$ and $L = 28$. Fat lines: Eq. 15. Inset: scaling close to $n_c(\Delta = 0) = 4$.

This determinant can be computed exactly [20]:

$$p_i = \prod_{j=1}^{L/2} \frac{2 \sin^2 \theta_j}{L+1} \prod_{k>j} 16 \sin^2 \left( \frac{\theta_j - \theta_k}{2} \right) \sin^2 \left( \frac{\theta_j + \theta_k}{2} \right)$$

and allows to go get $p_{\max}$: $p_{\max} = 2^{-L/2}$. The absence of a logarithmic term in $S_{n \to \infty} \sim -\ln p_{\max}$ is consistent with Eq. 7, because the contribution from the height shift exactly compensates for the Cardy-Peschel term at $R(\Delta = 0) = 1$. This also rigorously confirms at $\Delta = 0$ the value of $\delta$. We also checked the validity of Eq. 7 for the square lattice quantum dimer (2d-RK) wave function, for which $d = 1$. In this case the microscopic height representation of dimer coverings allows to obtain $\delta$ exactly at the lattice level.

*Conclusion.*— The Rényi-Shannon entropy of critical 1d systems does not only give a simple access to the Luttinger parameter of the system, it also shows that taking *powers* of the wave function gives rise to a whole line of critical points ending at a phase transition to an ordered state. In fact, going back to the 2d RK point of view, this transition reveals a rich structure in the entanglement spectrum $\{E_i\}$ of these 2d wave-functions. In some appropriate geometry [7] the probabilities $p_i$ are nothing else but the eigenvalues of the RK reduced density matrix and the probabilities directly give the entanglement spectrum $E_i = -\ln p_i$. The phase transition at $n_c$ shows that the spectrum has two sharply distinct regions in the thermodynamic limit: at high "energy" (small inverse "temperature" $n$) the universal contributions to the probabilities are Gaussian whereas at low energy (large $n$) they are dominated by the ordered configurations. This contrasts with the fractional quantum Hall situation where the universal part of the entangle-

ment spectrum only exist at low $E_i$ [21]. These findings may open new directions in the study of quantum critical wave-functions – in 1d and in higher dimensions – as well as their connection to boundary critical phenomena and $g$-factors in particular.

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[22] The winding numbers $W$ need not be summed over since only $W = 0$ contributes in the limit of infinite length in the imaginary time direction.
[23] $\mathcal{Z}^D$ is thus the square of the partition function a half-infinite cylinder (strip).
[24] A locking transition in the *bulk* is expected at $d^2 = 4\kappa r^2$. It however turns out that the latter does not affect Eq. 15, as confirmed by our numerical results. In the "book" picture and sufficiently far from the boundary it is indeed clear that all the pages (with a *fixed* stiffness $\kappa$) remain gapless in the bulk, whatever $n$.
[25] Such a behavior has already been observed in a dimer problem [7].